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Rotating wavepackets

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Abstract
Any free-particle wavepacket solution of Schrödinger's equation can be converted by differentiations to wavepackets rotating about the original direction of motion. The angular momentum component along the motion associated with this rotation is an integral multiple of $\hbar$. It is an *intrinsic* angular momentum: independent of origin and unchanged by Galilean boosts along the quantization direction. An example is given based on the three-dimensional Gaussian wavepacket, suitable for presentation to an undergraduate class on quantum mechanics.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Ohanian [1] has argued that spin is essentially a wave property, due to some kind of rotation within the wave. Unaware of Ohanian's paper, I showed that exact pulse solutions of Maxwell's equations can have an intrinsic angular momentum, unchanged by Lorentz boosts along the direction of net momentum of the pulse and invariant to change of spatial origin [2]. Likewise, acoustic pulses can carry angular momentum [3]. Here we show that any wavepacket solution of the free-particle Schrödinger equation

$$\mathrm{i}\hbar\partial_t\Phi = -\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)\Phi \tag{1}$$

can be converted by differentiations to wavepackets which rotate about their direction of motion. (By *wavepacket* we mean a localized normalizable function of space and time which satisfies (1).) Specifically, we consider net motion along the z-axis, so that the transverse momenta p_x and p_y have zero expectation values, and use cylindrical coordinates (ρ, ϕ, z) where $\rho^2 = x^2 + y^2$. Then (1) reads as

$$\mathrm{i}\hbar\partial_t\Phi = -\frac{\hbar^2}{2m}\left(\partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2}\partial_\phi^2 + \partial_z^2\right)\Phi \tag{2}$$

and the z-component of the angular momentum operator is

$$J_z = xp_y - yp_x = -\mathrm{i}\hbar(x\partial_y - y\partial_x) = -\mathrm{i}\hbar\partial_\phi. \tag{3}$$

Clearly Φ has to have azimuthal dependence for J_z to have non-zero expectation value. For example, the Gaussian wavepacket solution [4] of Schrödinger's equation,

$$\Phi_0(\rho, z, t) = (2\pi)^{-3/4}\left[b + \frac{\mathrm{i}\hbar t}{2mb}\right]^{-3/2} \exp\left\{\mathrm{i}k\left(z - \frac{1}{2}ut\right) - \frac{\rho^2 + (z-ut)^2}{4b\left[b + \frac{\mathrm{i}\hbar t}{2mb}\right]}\right\} \tag{4}$$

(where $u = \hbar k/m$) has no ϕ-dependence and $\langle J_z\rangle = 0$.

We shall first show how *any* free-particle solution which is independent of the azimuthal angle ϕ can be transformed into other exact solutions that do depend on ϕ and evaluate the resultant angular momentum. Then we shall use (4) to explicitly construct a spinning wavepacket.

2. Wavepackets which rotate about their direction of motion

Let Φ_0 be any solution of (1) which has no azimuthal dependence, not necessarily the Gaussian packet (4). The derivatives of Φ_0 with respect to x, y or z are also solutions of (1), as we can see by differentiating (1) with respect to any of x, y and z. Thus, for example,

$$\Phi_1 = (\partial_x + \mathrm{i}\partial_y)\Phi_0 \tag{5}$$

is a solution. Since

$$\partial_x = \cos\phi\,\partial_\rho - \frac{\sin\phi}{\rho}\partial_\phi, \qquad \partial_y = \sin\phi\,\partial_\rho + \frac{\cos\phi}{\rho}\partial_\phi, \tag{6}$$

we have

$$\partial_x + \mathrm{i}\partial_y = \mathrm{e}^{\mathrm{i}\phi}\left(\partial_\rho + \frac{\mathrm{i}}{\rho}\partial_\phi\right). \tag{7}$$

Hence, for Φ_0 independent of ϕ, (5) reduces to

$$\Phi_1 = \mathrm{e}^{\mathrm{i}\phi}\,\partial_\rho\Phi_0. \tag{8}$$

This solution of Schrödinger's equation is an eigenstate of J_z:

$$J_z\Phi_1 = \hbar\Phi_1. \tag{9}$$

Note that no assumptions have been made in deriving this result, which is independent of all of the parameters defining Φ_0, or indeed of its functional form. The eigenvalue is thus also unchanged by Galilean boosts along z (which, for example, change k and $u = \hbar k/m$ in (4)). Thus $\langle J_z\rangle_1 = \hbar$ holds in all frames, including the 'rest' (zero-momentum) frame, and can be regarded as an *intrinsic* angular momentum.

Likewise the operator $\partial_x - \mathrm{i}\partial_y = \mathrm{e}^{-\mathrm{i}\phi}\left(\partial_\rho - \frac{\mathrm{i}}{\rho}\partial_\phi\right)$ will produce a rotating packet with eigenvalue $-\hbar$ for J_z. Higher $\langle J_z\rangle$ values can be obtained by more differentiation:

$$\Phi_2 = (\partial_x + \mathrm{i}\partial_y)^2\Phi_0 = (\partial_x + \mathrm{i}\partial_y)\Phi_1 = \mathrm{e}^{\mathrm{i}\phi}\left(\partial_\rho + \frac{\mathrm{i}}{\rho}\partial_\phi\right)\mathrm{e}^{\mathrm{i}\phi}\,\partial_\rho\Phi_0 = \mathrm{e}^{2\mathrm{i}\phi}\left(\partial_\rho^2 - \frac{1}{\rho}\partial_\rho\right)\Phi_0 \tag{10}$$

has $\langle J_z\rangle_2 = 2\hbar$ and so on. In general, for $\Phi_n = (\partial_x \pm \mathrm{i}\partial_y)^n\Phi_0$, the eigenvalue of J_z is $\pm n\hbar$.

At this point the quantum mechanics class might be invited to show that Φ_1 is not an eigenstate of J_x or of J_y, but that $\langle J_x\rangle_1 = 0 = \langle J_y\rangle_1$ etc, and to experiment with other derivatives. For example, the wavepacket based on $\partial_x\Phi_0$ has zero expectation value for all components of $\mathbf{J}$. Likewise, the combination $(\partial_x + \mathrm{i}\partial_y)(\partial_x - \mathrm{i}\partial_y) = \partial_x^2 + \partial_y^2 = \partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2}\partial_\phi^2$ operating on $\tilde{\Phi}_0$ produces a wavepacket without azimuthal dependence and thus with zero $\langle J_z\rangle$.

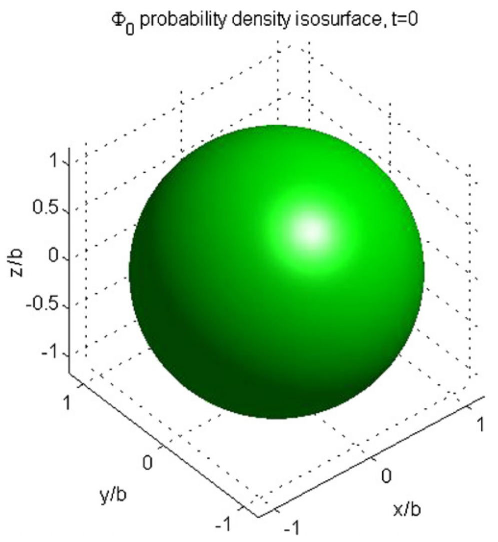

Figure 1. Probability density isosurface of Φ_0, shown at one-half of its maximum value at $t = 0$. The isosurfaces are spheres. At $t = 0$ the packet is at its most compact, with $\langle r^2 \rangle = 3b^2$. The packet is in motion upward along the z-axis, and will expand as it propagates: $\langle r^2 \rangle_t = 3b^2 + (k^2 + \frac{3}{4b^2})(\frac{\hbar t}{m})^2$.

Clearly, a procedure which gives integer spin cannot describe the electron. The usual route to spin $\frac{1}{2}$ is via a relativistic formulation (the Dirac equation), as discussed in most quantum mechanics texts. However, the key step is actually the *linearization* of the Schrödinger equation [5], namely the derivation of an equation which is linear in the spatial as well as the time derivatives. This results in a four-component (spinor) wavefunction for a spin $\frac{1}{2}$ particle, with the correct g-factor, in a completely non-relativistic formulation.

3. A rotating wavepacket based on the Gaussian pulse

We shall consider the properties of the wavepacket $\Phi_1 = e^{i\phi}\partial_\rho \Phi_0$, where now Φ_0 has the Gaussian form (4). Differentiation with respect to ρ introduces the factor $\frac{-\rho}{2b[b+i\hbar t/2mb]}$. Thus Φ_1 is a hollow pulse, with zero probability amplitude on the z-axis ($\rho = 0$). In addition, Φ_1 has the $e^{i\phi}$ azimuthal dependence, and angular momentum density equal to $\hbar$ times the probability density:

$$2b^2 \Phi_1^* (-i\hbar \partial_\phi) \Phi_1 = \hbar 2b^2 |\partial_\rho \Phi_0|^2 \tag{11}$$

(The factor $2b^2$ is inserted because $\int d^3r |\Phi_1|^2 = 1/2b^2$; note that Φ_0 is normalized to unity, $\int d^3r |\Phi_0|^2 = 1$.) Thus, the probability density and angular momentum density are both zero on the axis of symmetry. Figure 1 shows $|\Phi_0|^2$, while figure 2 shows $|\Phi_1|^2$, in both cases at one-half of their maximum values.

It is interesting to compare key expectation values obtained for the wavepackets Φ_0 and Φ_1, listed on the left- and right-hand sides in the following:

$$\langle J_z \rangle_0 = 0, \qquad \langle J_z \rangle_1 = \hbar, \tag{12}$$

$$\langle p_z \rangle_0 = \hbar k, \qquad \langle p_z \rangle_1 = \hbar k, \tag{13}$$

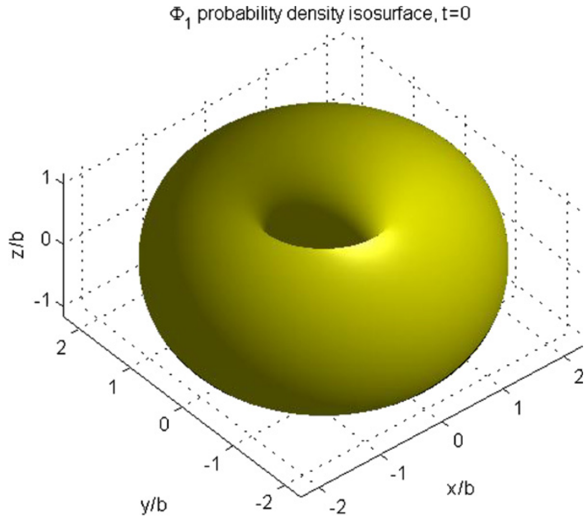

Figure 2. Probability density isosurface of Φ_1, at one-half of $|\Phi_1|^2_{\max}$ at the focal point ($t = 0$). The packet is hollow on the symmetry axis. At earlier or later times the packet is larger: $\langle r^2\rangle_t = 5b^2 + (k^2 + \frac{5}{4b^2})(\frac{\hbar t}{m})^2$. In addition to the vertical motion of the wavepacket, there is circular motion about the z-axis.

$$\langle p_z^2\rangle_0 = \hbar^2\left(k^2 + \frac{1}{4b^2}\right), \qquad \langle p_z^2\rangle_1 = \hbar^2\left(k^2 + \frac{1}{4b^2}\right) \tag{14}$$

$$\langle p^2\rangle_0 = \hbar^2\left(k^2 + \frac{3}{4b^2}\right), \qquad \langle p^2\rangle_1 = \hbar^2\left(k^2 + \frac{5}{4b^2}\right), \tag{15}$$

$$\langle \rho^2\rangle_0 = 2b^2 + \frac{\hbar^2 t^2}{2m^2b^2}, \qquad \langle \rho^2\rangle_1 = 4b^2 + \frac{\hbar^2 t^2}{m^2b^2}, \tag{16}$$

$$\langle z^2\rangle_0 = b^2 + \frac{\hbar^2}{m^2}\left(k^2 + \frac{1}{4b^2}\right)t^2, \qquad \langle z^2\rangle_1 = b^2 + \frac{\hbar^2}{m^2}\left(k^2 + \frac{1}{4b^2}\right)t^2. \tag{17}$$

Both Φ_0 and Φ_1 represent wavepackets that move at group velocity $\mathbf{u} = (0, 0, \hbar k/m)$: both have

$$\langle \mathbf{r}\rangle = (\langle x\rangle, \langle y\rangle, \langle z\rangle) = (0, 0, \hbar kt/m). \tag{18}$$

Both reach their focal region centred on $\mathbf{r} = 0$ at $t = 0$. For the same parameters k and b, Φ_0 and Φ_1 have the same longitudinal spread, as measured by the mean-square deviation in z:

$$(\Delta z)^2 = \langle z^2\rangle - \langle z\rangle^2 = b^2 + \left(\frac{\hbar}{2mb}\right)^2 t^2. \tag{19}$$

From (13) and (14) we have $(\Delta p_z)^2 = \langle p_z^2\rangle - \langle p_z\rangle^2 = \hbar^2/4b^2$, so that the longitudinal uncertainty product is the same for both Φ_0 and Φ_1:

$$\Delta z \Delta p_z = \frac{\hbar}{2}\sqrt{1 + \left(\frac{\hbar t}{2mb}\right)^2}. \tag{20}$$

As expected, Φ_1 has the larger transverse spread: from (15) we see that $\langle \rho^2\rangle_1 = 2\langle \rho^2\rangle_0$ for the same values of k, b and t. The main difference lies in the azimuthal flow: Φ_1 has an azimuthal component in its probability density current, proportional to $\mathrm{Im}(\Phi_1^* \nabla \Phi_1)$. From (11) this is proportional to $\rho^{-1}|\partial_\rho \Phi_0|^2$.

4. Discussion

We have seen how any free-particle wavepacket solution of the Schrödinger equation can be converted by differentiations to rotating wavepackets, which have angular momentum component along the direction of motion equal to an integer multiple of $\hbar$. (When seen in their zero-momentum frames, the wavepackets still have an axis of symmetry, here the z-axis, and thus we do not need motion to define the preferred direction.)

An example, based on Darwin's Gaussian wavepacket (4), is discussed in detail. There is ample opportunity for class projects, for instance study of wavepackets with higher angular momenta, $\Phi_n = (\partial_x + \mathrm{i}\partial_y)^n \Phi_0$. After Φ_1 given by (8) the first few of these are, assuming as before that Φ_0 is independent of ϕ,

$$\Phi_2 = \mathrm{e}^{2\mathrm{i}\phi}\left(\partial_\rho^2 - \frac{1}{\rho}\partial_\rho\right)\Phi_0, \tag{21}$$

$$\Phi_3 = \mathrm{e}^{3\mathrm{i}\phi}\left(\partial_\rho^3 - \frac{3}{\rho}\partial_\rho^2 + \frac{3}{\rho^2}\partial_\rho\right)\Phi_0, \tag{22}$$

$$\Phi_4 = \mathrm{e}^{4\mathrm{i}\phi}\left(\partial_\rho^4 - \frac{6}{\rho}\partial_\rho^3 + \frac{15}{\rho^2}\partial_\rho^2 - \frac{15}{\rho^3}\partial_\rho\right)\Phi_0. \tag{23}$$

Among the relations to be checked in the calculation of expectation values is that (for example) $\langle p_z \rangle$ and $\left\langle p_z^2 \right\rangle$ are independent of time, while $\langle z^2 \rangle$ depends quadratically on time (see [6] for a derivation),

$$\langle z^2 \rangle_t = \langle z^2 \rangle_0 + \frac{(\Delta p_z)^2}{m^2} t^2, \tag{24}$$

where $(\Delta p_z)^2 = \left\langle p_z^2 \right\rangle - \langle p_z \rangle^2$ is the mean-square deviation in p_z.

We note finally that there are many parallels between the quantum particle case, discussed here, and the electromagnetic and acoustic cases [2, 3]. One notable difference is that the vector electromagnetic field can have angular momentum even in the absence of azimuthal dependence in the pulse solution of the wave equation on which it is based [2]. Of course, the unquantized electromagnetic and acoustic wavepackets can have any value of $\langle J_z \rangle$.

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